Systematic methods for synthesis and design of sustainable chemical and biochemical processes

Gani, Rafiqul

Publication date:
2011

Document Version
Publisher's PDF, also known as Version of record

AMIDIQ

ACADEMIA MEXICANA DE INVESTIGACIÓN Y DOCENCIA EN INGENIERÍA QUÍMICA, A.C.

XXXII Encuentro Nacional y 1er Congreso Internacional

"La Ingeniería Química en el Año Internacional de la Química"

Eventos:

- Conferencias plenarias
- Sesiones orales
- Exposiciones de carteles
- Talleres
- Feria de posgrado y exposición industrial

International Year of CHEMISTRY 2011

3 al 6 de mayo de 2011

Riviera Maya, Q.R.

Secretaría de Turismo Quintana Roo 2005 2011 | SEDETUR

Riviera Maya www.rivieramaya.com

GRUPO ACF

CONACYT 40 años

Casa abierta al tiempo

COMECYT

FICSAC

- **11:00-12:00 hrs**

Sesión Plenaria

Systematic methods for synthesis and design of sustainable chemical and biochemical processes

Rafiqul Gani
CAPEC, Department of Chemical & Biochemical Engineering
Technical University of Denmark

Chemical and biochemical process design consists of designing the process that can sustainably manufacture an identified chemical product through a chemical or biochemical route. The chemical product tree is potentially very large; starting from a set of basic raw materials (such as petroleum, biomass, coal, natural gas, rock, *etc.*, that are usually extracted), to a bigger set of basic chemical products (such as, ethylene, benzene sulfuric acid, ammonia, *etc.*, that are produced in large quantities), to an even bigger set of intermediates (such as, methanol, urea, succinic acid, ethylene glycol, *etc.*, that are produced from the basic chemicals), to a very large number of refined chemicals and consumer products (where the chemical selected as the active ingredient is usually used in small quantity). At the top, the chemical products are usually from the life sciences, pharmaceutical, food and related industries and their development is principally based on experiment-based trial and error approaches. At the lower-middle end, the chemical products usually from the oil, petrochemical and chemical industries and use of model based tools in their development is quite common. Using raw materials from the renewable resources, the sustainability of the product and therefore the process can be improved. Also, the number of alternatives that exist provide opportunities and challenges to find the best synthesis routes, for example, for process intensification or a multi-product processing complex like a biorefinery.

The process synthesis design problem can be formulated as one where first a synthesis-design target (a process with desired qualities) is defined and then design alternatives (process flowsheets for different raw material-product connection) that match the target are identified and ordered according to a performance index. One way to achieve this, is to derive a generic mathematical formulation of the synthesis-design problem and then to decompose it into a set of easily manageable and solvable sub-problems. The sub-problems are solved according to a hierarchy that gradually decreases the number of feasible alternatives. The final step involves solving a well-defined optimization problem or simply ordering the feasible solutions according to defined performance

criteria to determine the optimal solution. This synthesis-design approach is suitable for problems that are highly non-linear, contain models and data from different sources, has a large combinatorial problem size, and/or require the use of multiple methods and tools.

The decomposition based "define target – match target" approach to process synthesis-design has been converted into model-based computer-aided tools for process intensification, sustainable process design, identification of optimal biorefinery models as well as integrated process-control design, and chemical product design. The lecture will present the main concepts, the decomposition based solution approach, the developed methods and tools together with illustrative examples covering chemical and biochemical process synthesis and design.

- **12:00-13:00 hrs**
  Clausura